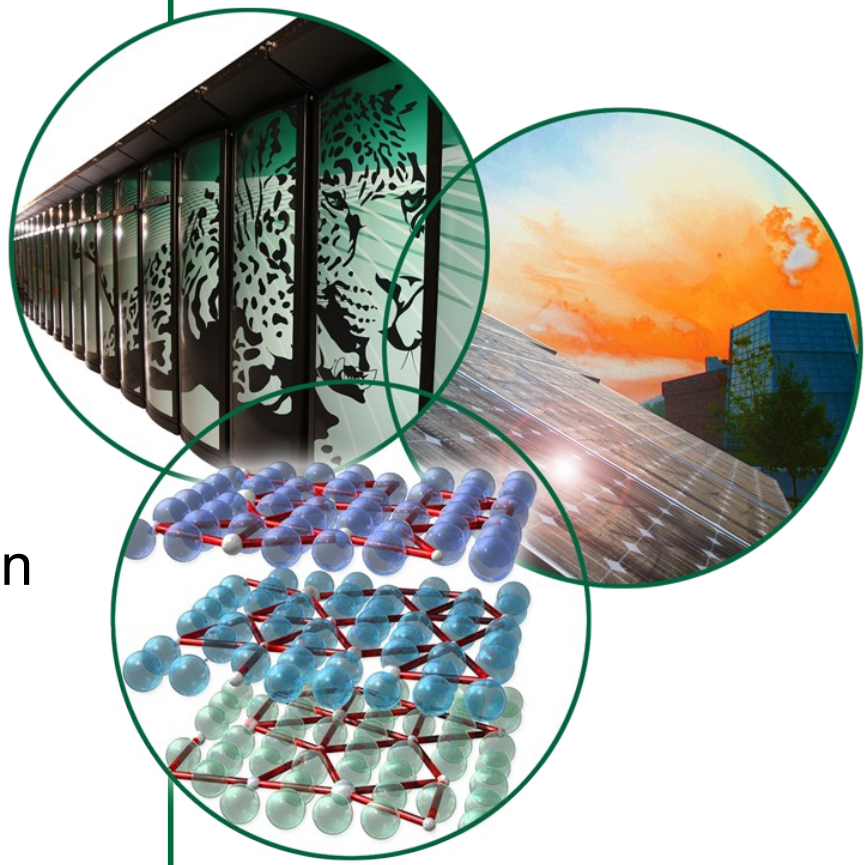
Multi-Tiered Separations Process Modeling



Valmor de Almeida

Nuclear Science & Technology Division

DOE-NE Germantown MD
02 October 2009

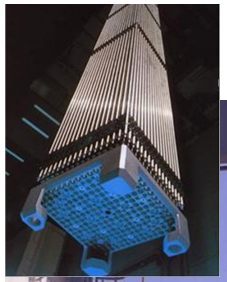
U.S. DEPARTMENT OF ENERGY

NEAMS PI Meeting

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

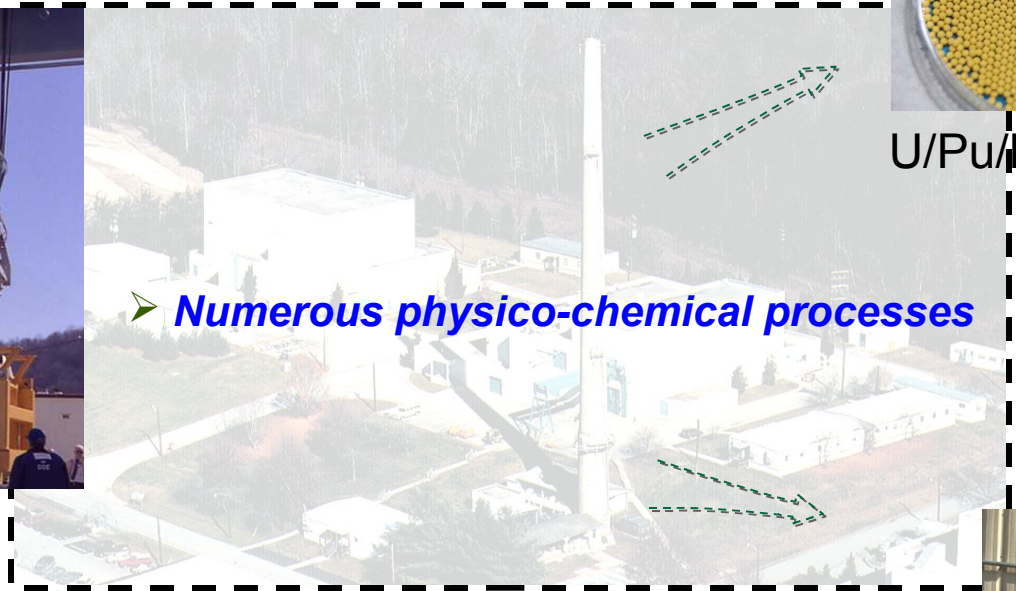
The separations domain is the entire reprocessing plant

Spent Nuclear Fuel



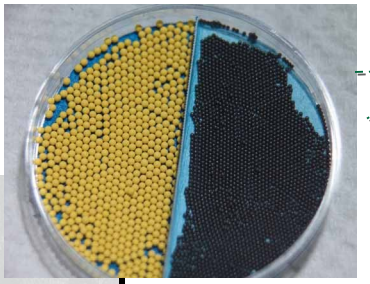
fuel receiving

Reprocessing Plant



- ***Numerous physico-chemical processes***

Product Forms



U/Pu/Np forms

Fuel Fab

Waste Disposal

Waste Forms

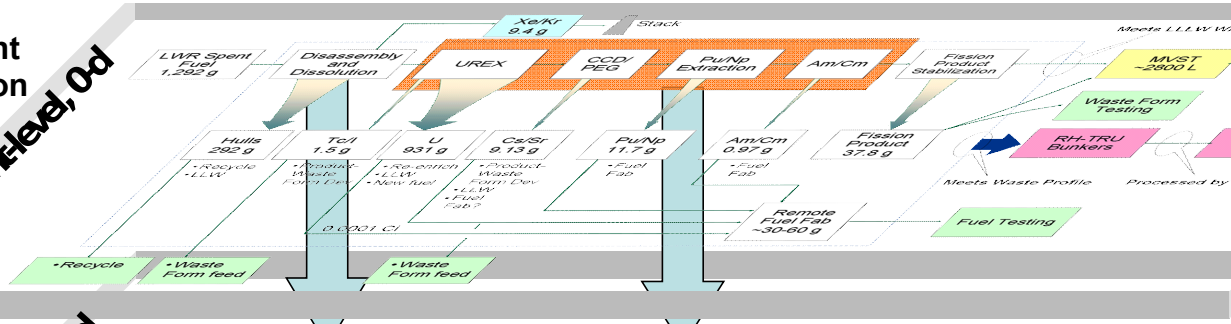
- ***High efficiency & robustness***
- ***High quality fuel product***
- ***Minimum waste & effluents***
- ***Minimum environmental impact***
- ***Minimum proliferation concerns***

M&S for all separation processes fit a multi-tiered approach

A primary goal is the development of an integrated plant model that allows dynamic simulations of the operation of separations plants and integrated safeguards of various configurations and operating conditions. Subscale models to provide required fidelity in chemical and physical processes.

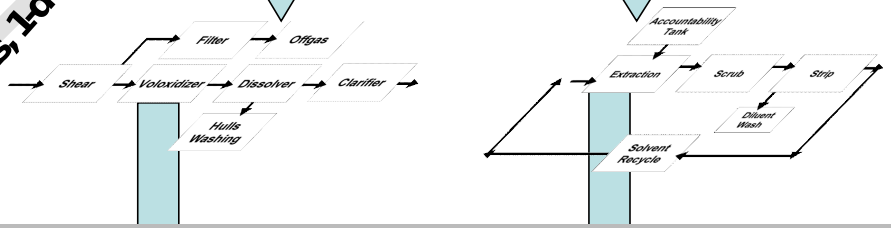
Process development
Design and evaluation
Safety analysis

Plant-level, 0-d



Unit operations, 1-d

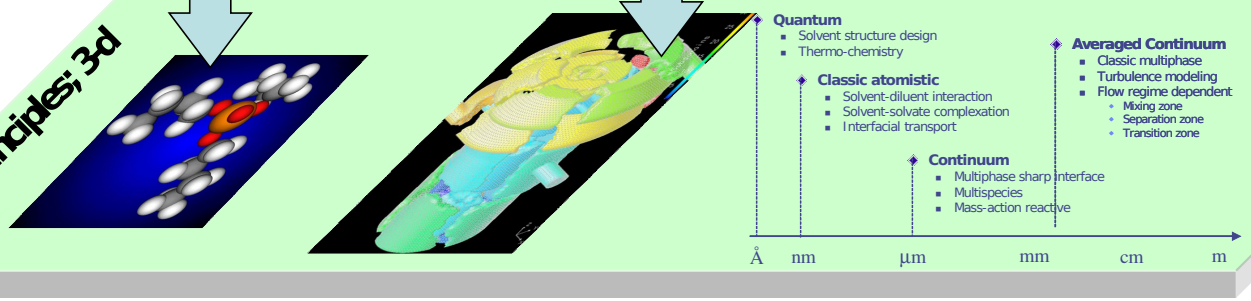
Equipment design
Safety



Requirements at plant level drive development of unit operations and subscale models

First-principles, 3-d

Agent design
Thermodynamics
Transport

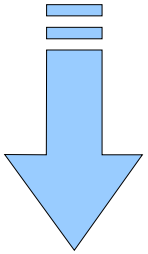


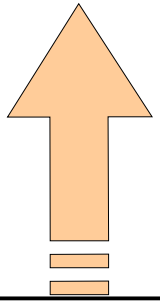
Implementation activities focused on long-term vision while addressing short-term user needs

1) Plant-level simulation toolkit

- Community consensus this is a priority
- Needed to define the bottom-up work

Top-down





Bottom-up

2) Ligand molecular design for solvent extraction

- Robust trivalent minor actinides separation is a challenge
- A major focus of the FCR&D Separations and Waste Form campaign (Sigma team) is to separate Am/Cm

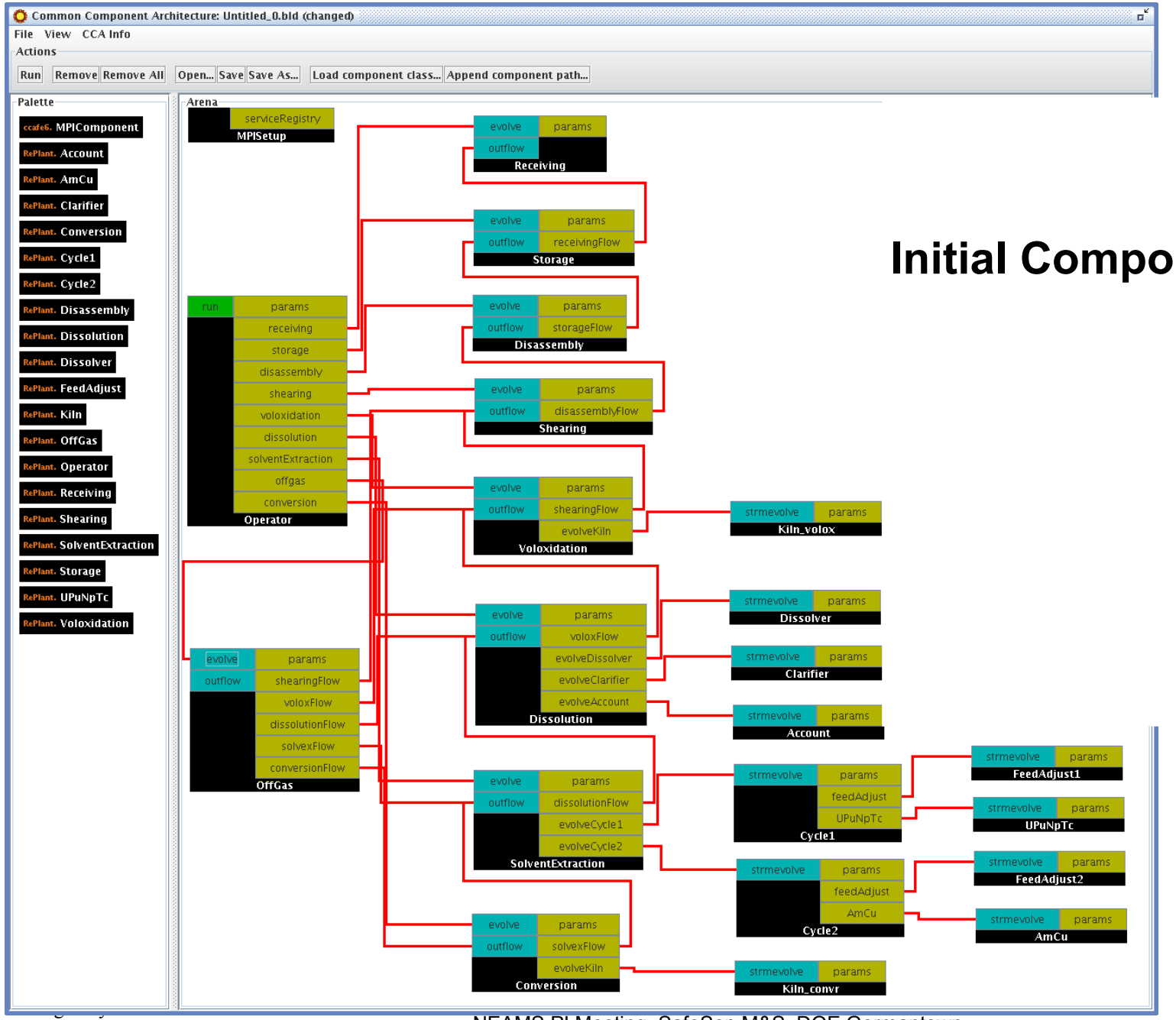
1) Plant-level IPSCs Strategy

- **10-Yr Vision**
  - A digital reprocessing plant

- **Initial Requirements**
  1) Leverage legacy unit ops codes in all major languages
     - Minimum code modification to turn them into libraries
  2) Use existing scientific software composition framework
  3) Open & closed source integration and development
  4) Support safeguards by design approach
  5) Enable parallel computing

- **Progress**
  - Tested CCA-tools (SciDAC) viability:
    - Adopted the CCA specification
    - Used Ccaffeine framework to compose a plant-level application
    - Took advantage of Babel's language interoperability through SIDL

CCA-based Plant-level Simulation



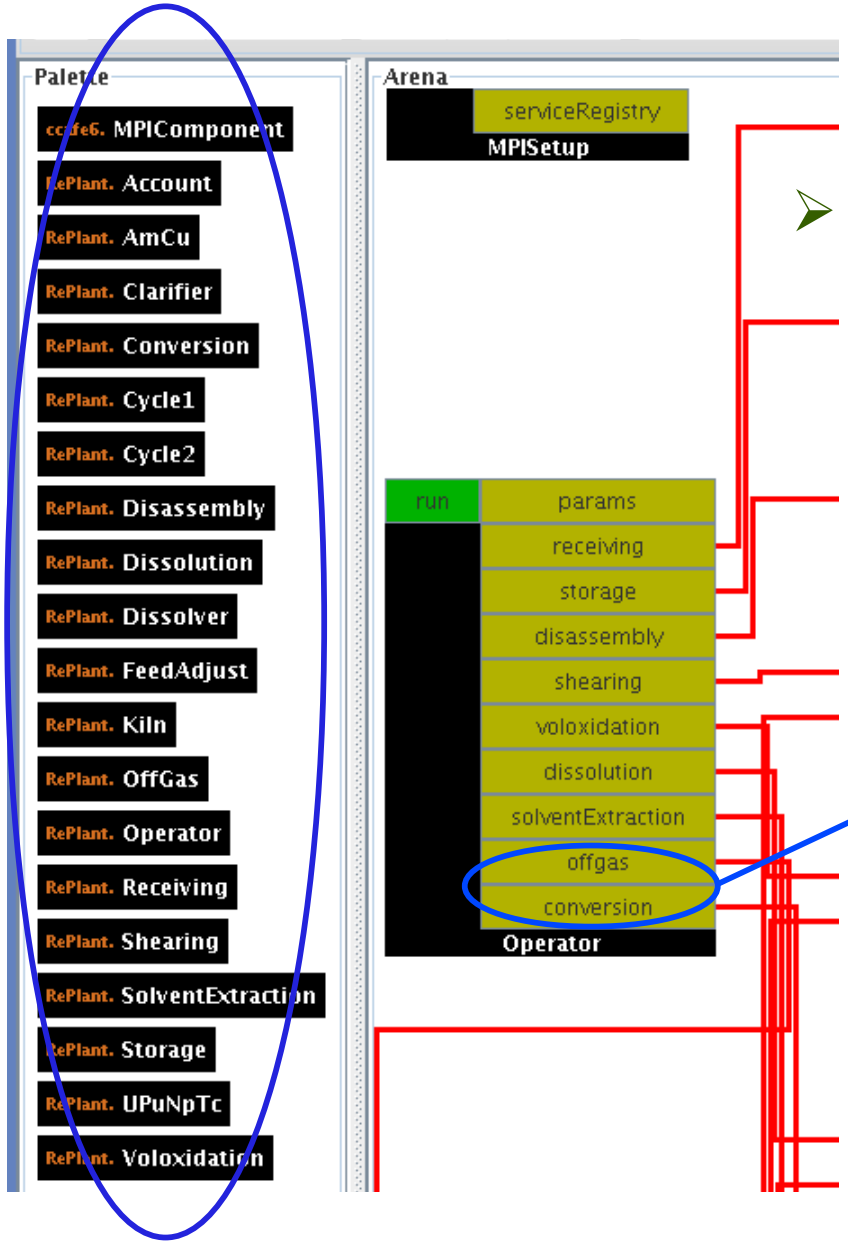
Initial Component Design

An Initial Plant Toolkit

19 components

3 ports

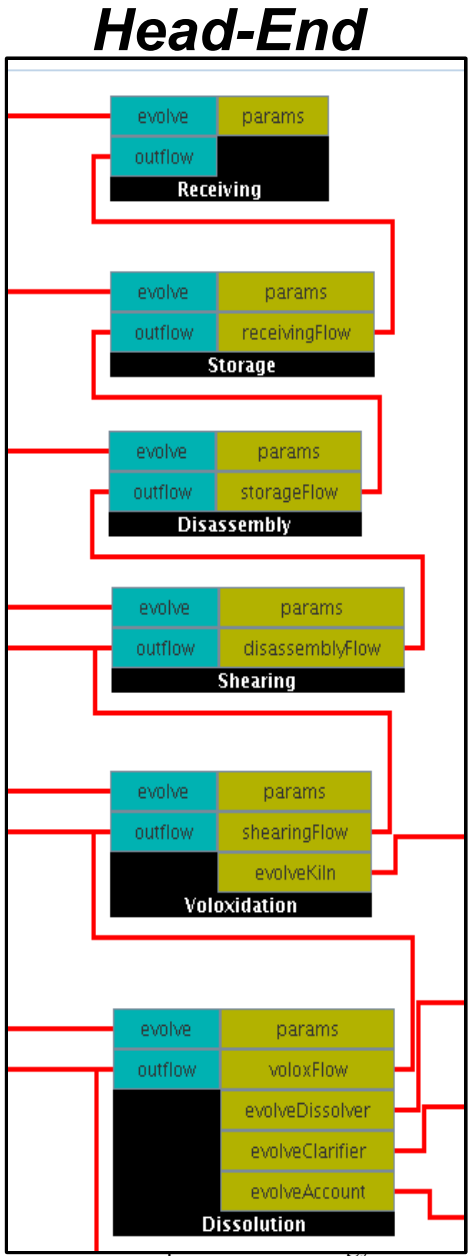
1 interface

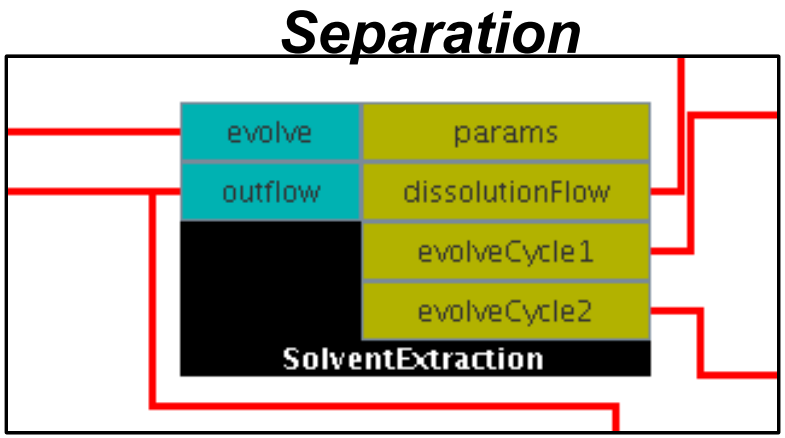


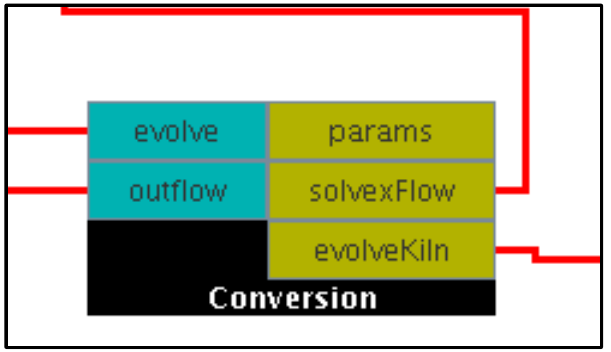
- **Operator**
  - Algorithm logic
  - Time advance the major components of the plant
  - Interrupt simulation gracefully
  - Little private data (“alerts”)
  - Currently, time evolution is ordered according to “uses” port connectivity, e.g. :

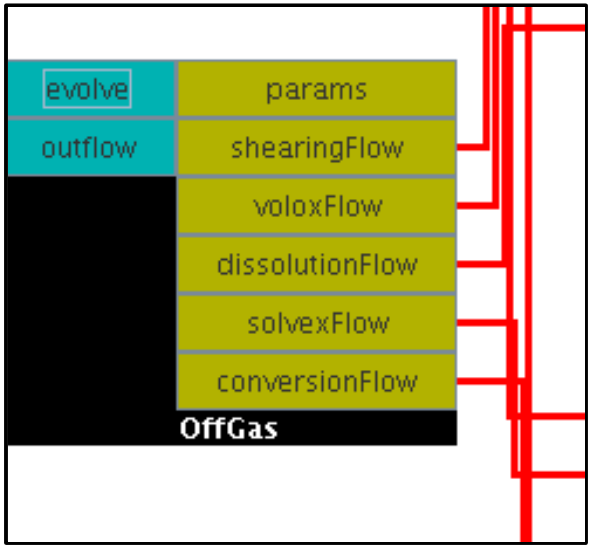
“Conversion” needs to be time-advanced before “OffGas”

Plant toolkit sub-systems represent major sections of a plant



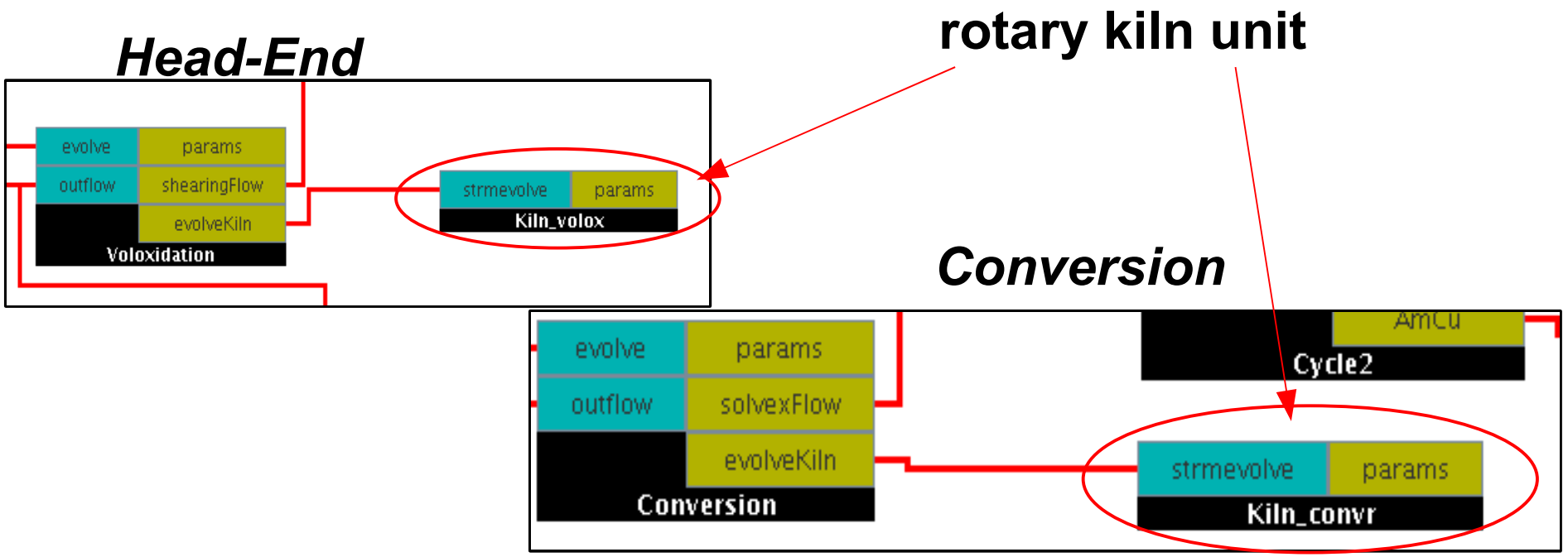




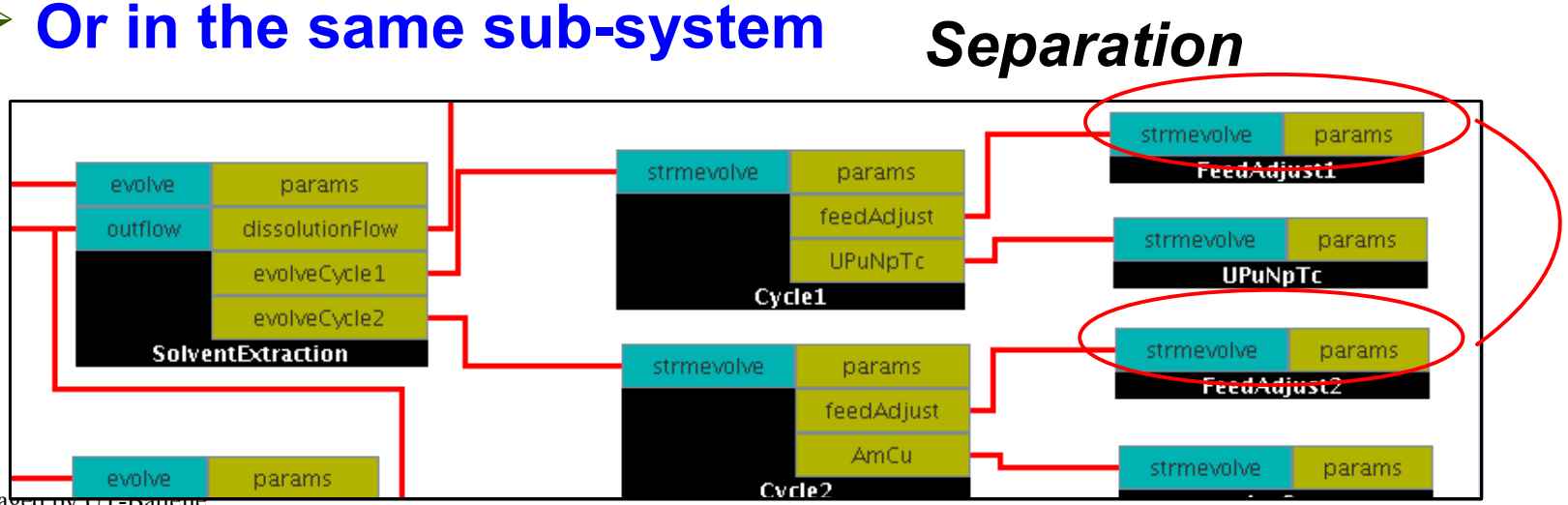


- **Components at this level perform sub-system algorithm logic and hold data**

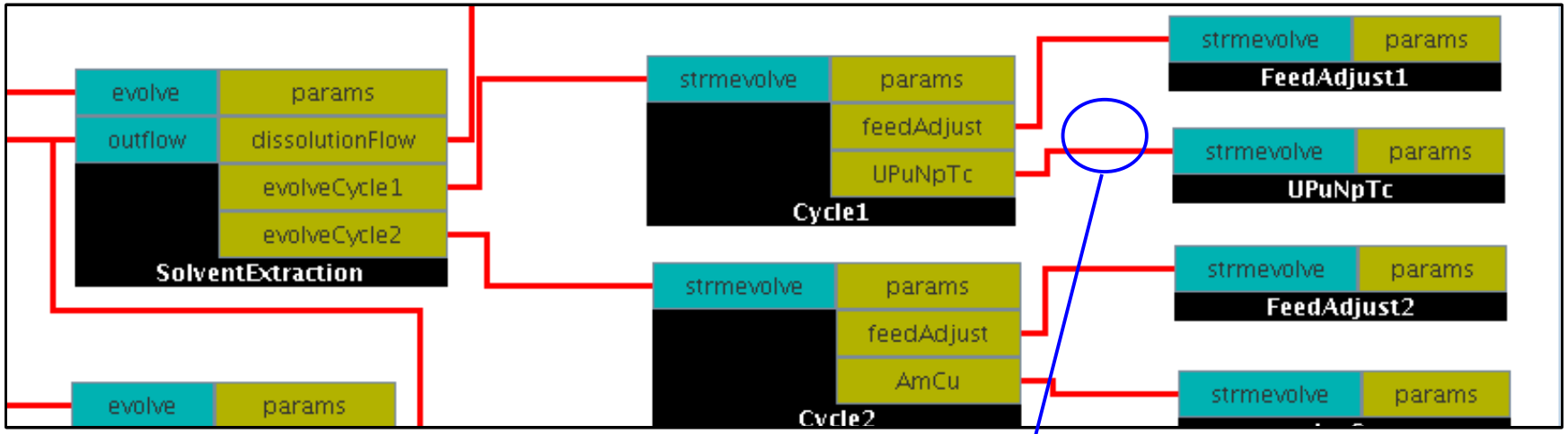
Components can be instantiated multiple times in different sub-systems



- Or in the same sub-system

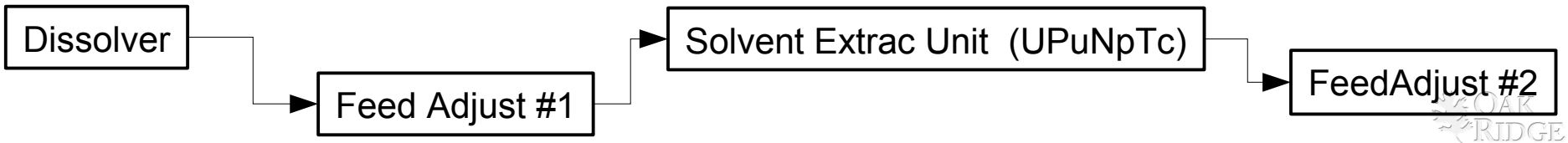


Workflow and Material (data) Flow Differ

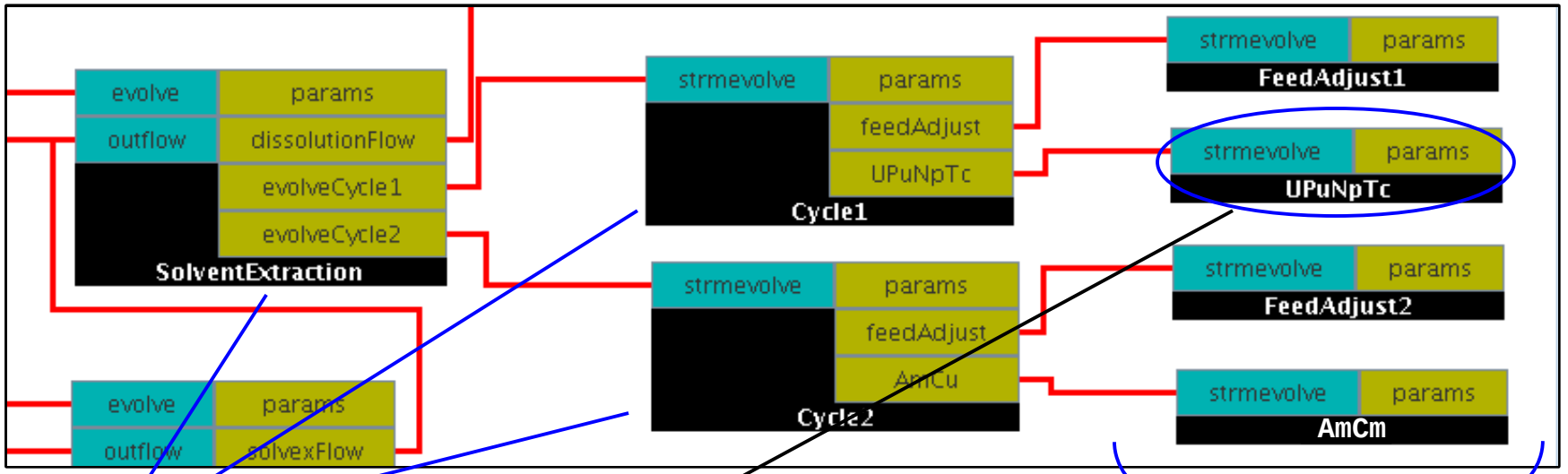


The solvent extraction Cycle1 calls a method in UPuNpTc and data flows both ways

```
package RePlant version 0.0 {
    interface StreamsEvolver extends gov.cca.Port
    {
      array< MaterialStream >
      TimeAdvance( in double timeInterval, in double timeStamp,
                   in array< MaterialStream > inFlowStreams );
    }
}
```



Unit Ops Code Development Approach

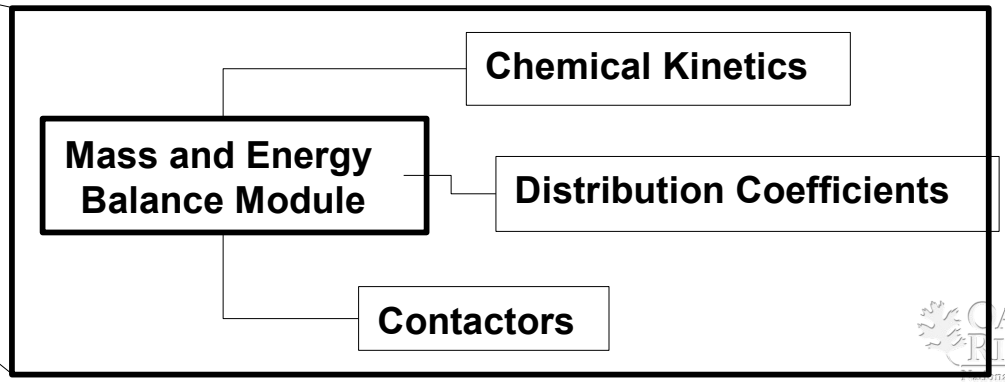


algorithm logic

library wrappers

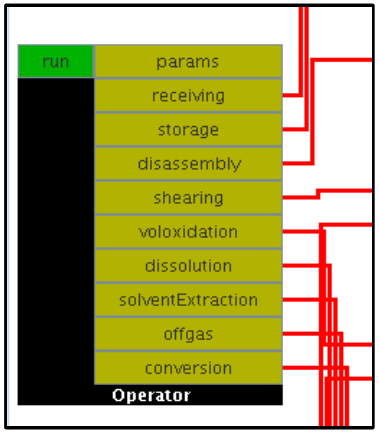
underlying library

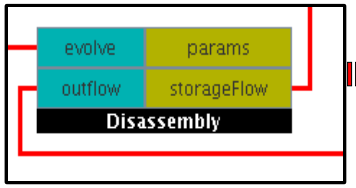
Solv. Extr. Contactor Bank



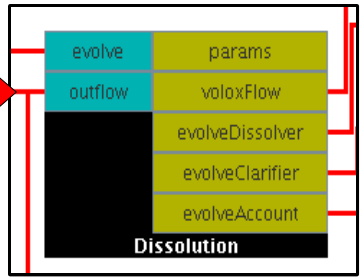
leverage of SEPHIS ORNL code written in the 70's

Preliminary Verification

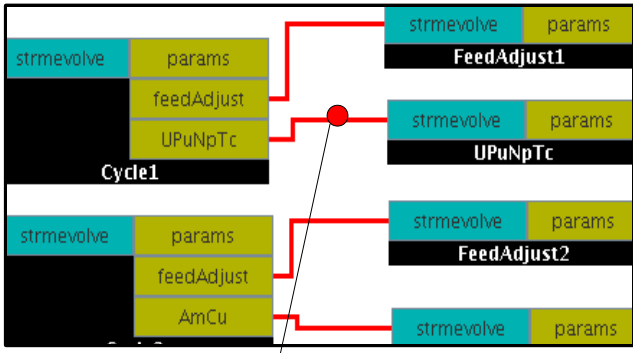


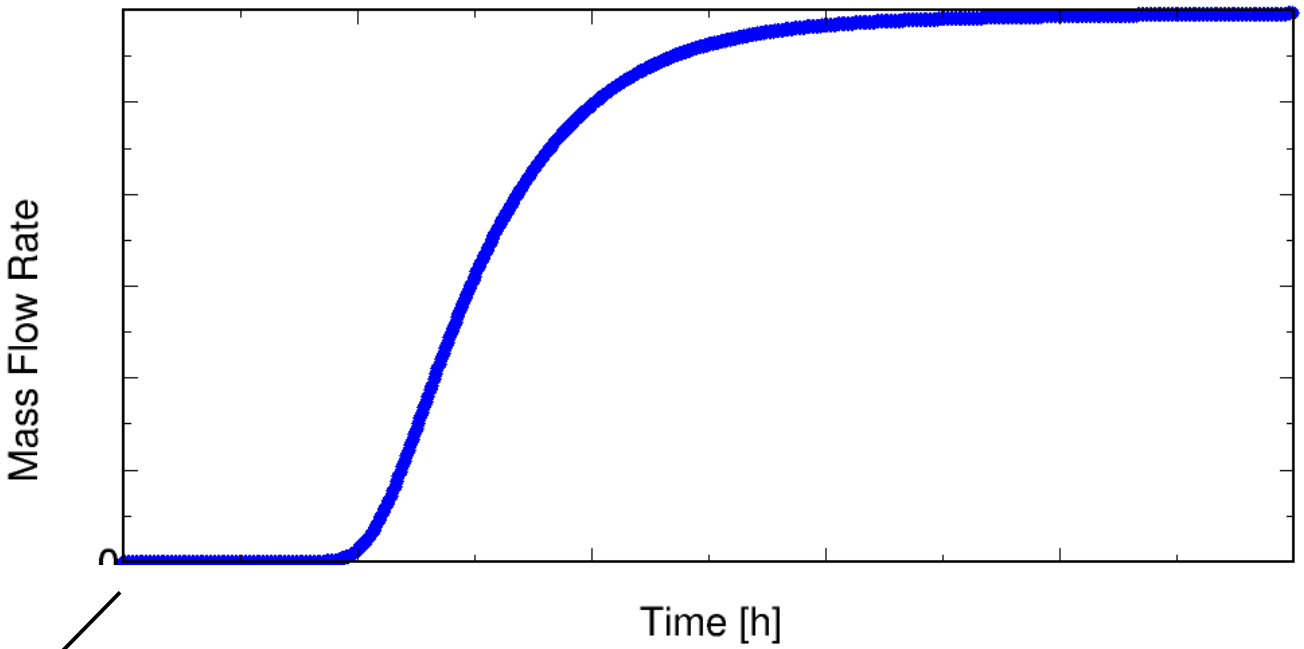


assembly



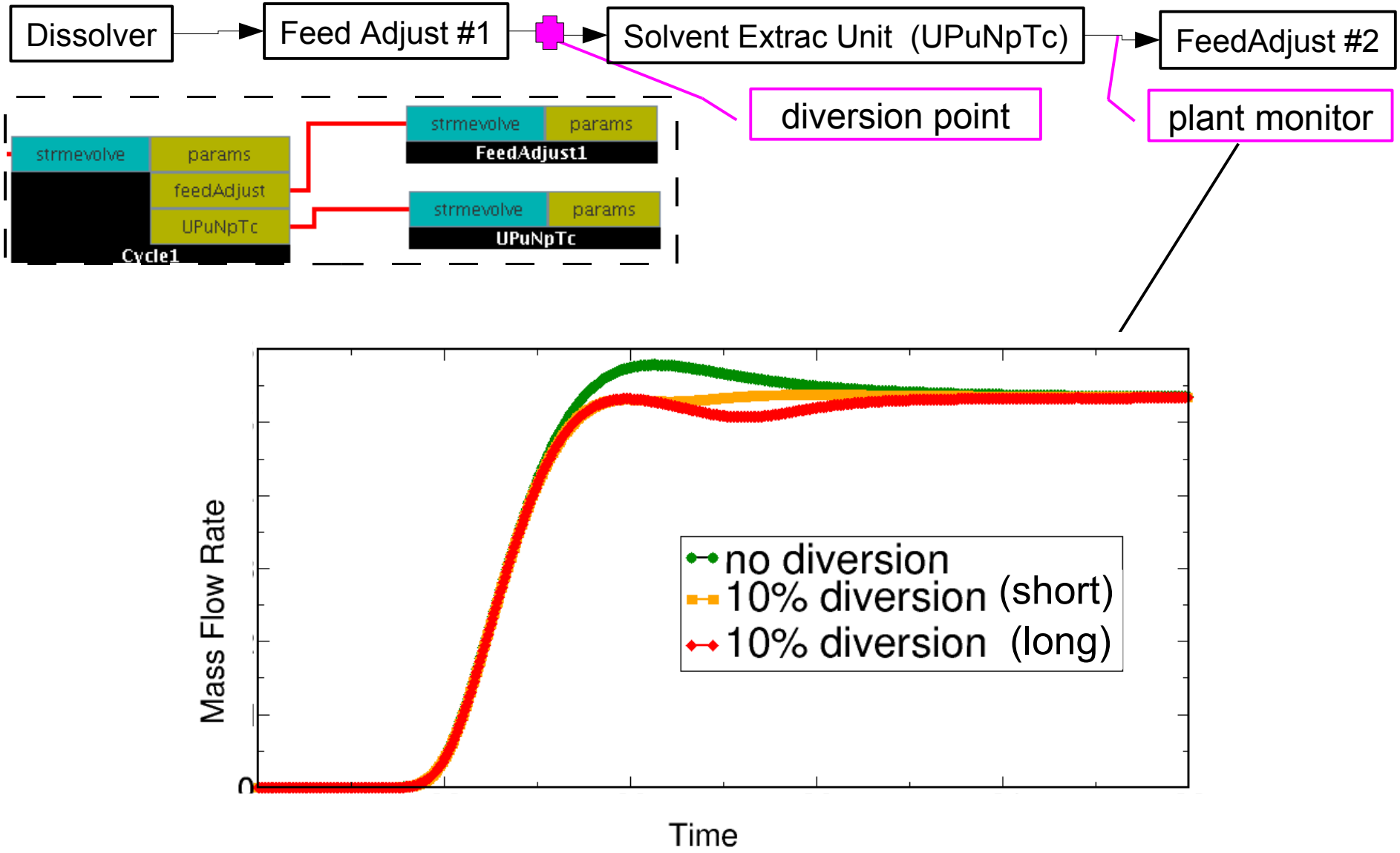
feed





feed enters solvent extraction unit

A Diversion Test for Safeguards



2) Ligand Design IPSCs Strategy

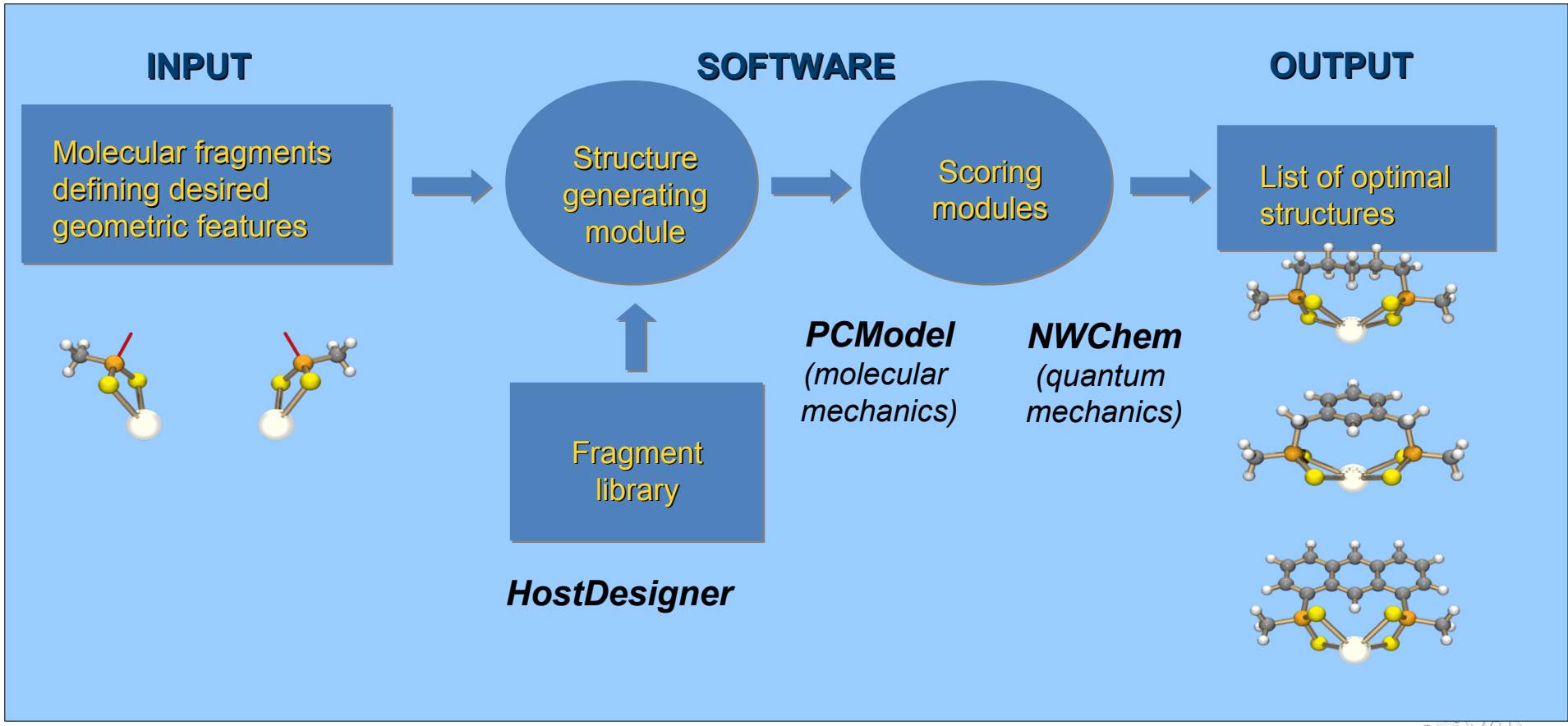
- **10-Yr Vision**
  - Solvent extraction molecular design

- **Initial requirements**
  1) Parallelize the HostDesigner code (ORNL; Ben Hay)
  2) Extend to incorporate computational quantum mechanics

- **Progress**
  - MPI parallelization
  - Code modifications in preparation for QM extensions

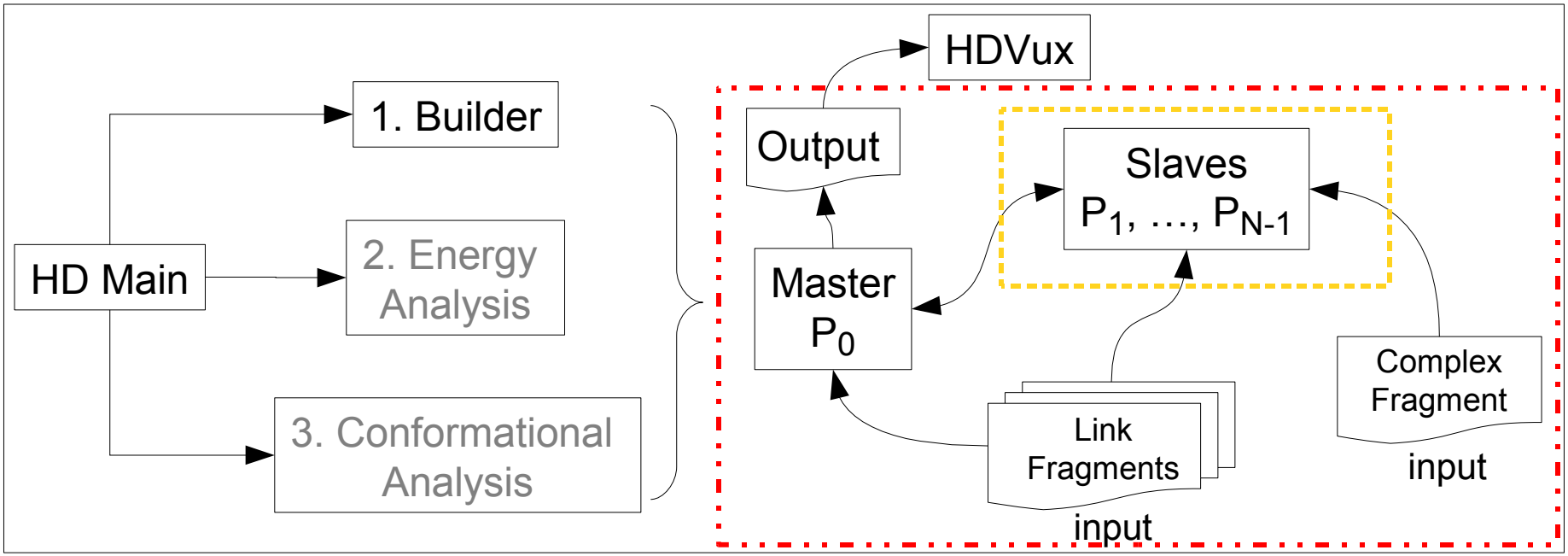
New ligands for selective complexation of metal ions (HostDesigner)

Computer-aided, structure-based design of radionuclide sequestering agents is being used to guide experimental programs. Increase in fragment library size and need for more accurate scoring motivates adapting this system for supercomputers.



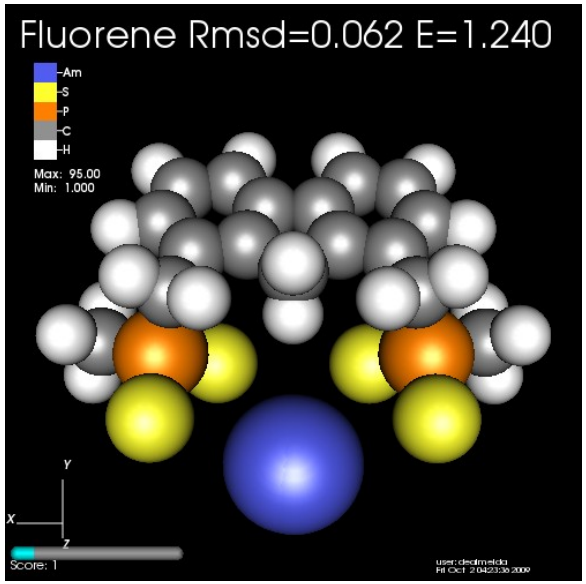
Progress on Parallelization

- Parallelization of Host-Designer active items
  - Master-slave approach for balancing the computational work
  - Planning parallel IO



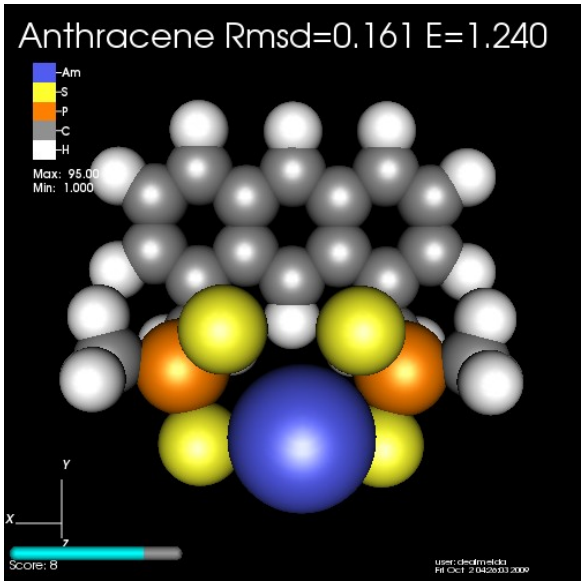
Verification against sequential code results

- Americium dimethylphosphinate chelate complex fragment



asymmetric

candidates



1st candidate

8th candidate

- Parallel results match sequential code
- Ligand suggested for synthesis by Minor Actides Sigma Team

Speed-up Results in Development

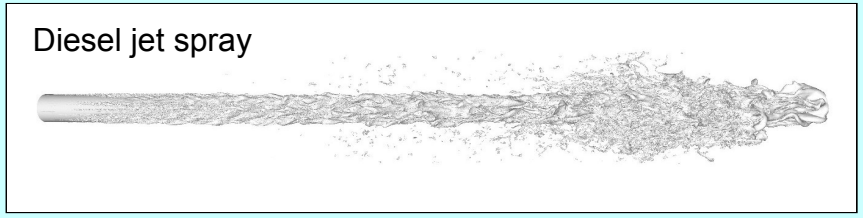
Library – 966 418 Links			
# Proc's	Build [s]	Speedup	# Trial Links
1	108.4	-	39 685
2	55.2	2	19 842
4	38.6	3	9 921
8	24.2	4	4 961
16	13.4	8	2 480
32	7.1	15	1 240
64	3.5	31	620

- Load balance not fully implemented (I/O dependent)

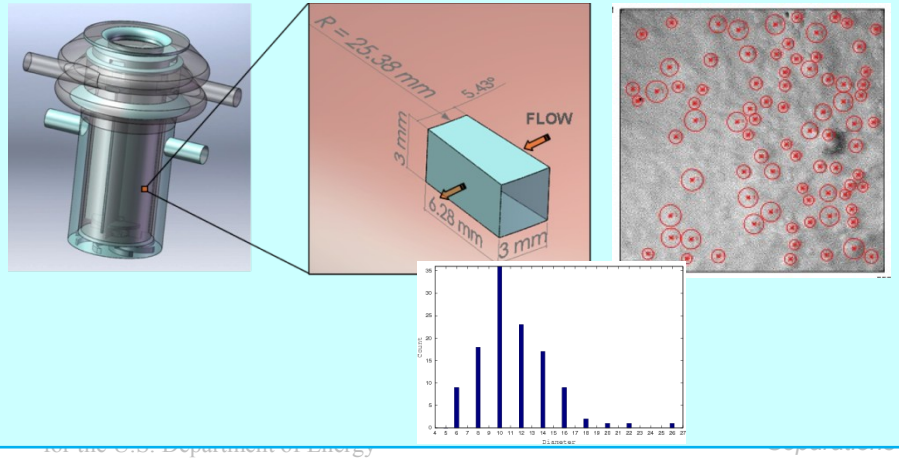
Related Actvities

- **Sharp Interface Tracking in Rotating Microflows of Solvent Extraction – NEUP award AFCI 09-349 (DOE NE Sponsor)**
  - State University of New York at Stony Brook and ORNL collaboration to model microscale drop behavior in centrifugal contactors

- **SUNY-SB has unique expertise in interface tracking**

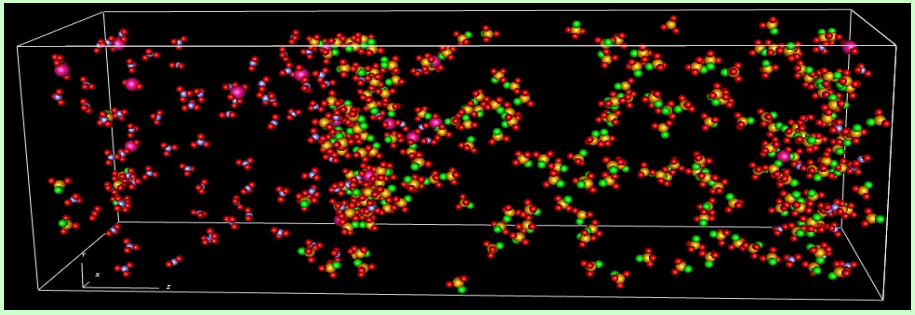


- **ORNL will provide modeling insight and data**

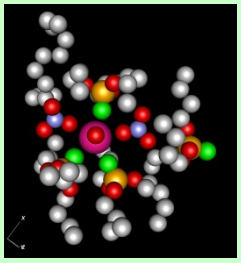


- **Quantifying Water Extraction by TBP/Dodecane via Molecular Dynamics Simulation - NEUP award AFCI 09-430 (NNSA NA-24 sponsor)**
  - University of Tennessee at Knoxville and ORNL collaboration to model molecular interfacial transport in solvent extraction

- **UTK and ORNL worked on uranyl extraction (JDRD/LDRD effort FY:07-08)**

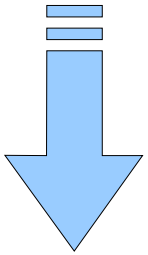


- **ORNL will provide modeling insight and data**
  - **QM-derived electrostatic potentials**
  - **Water absorption in TPB-dodecane**



Outlook

Top-down

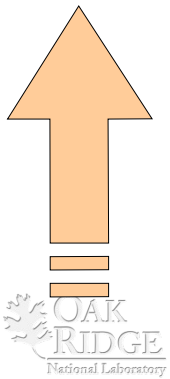


- Expand CCA plant-level application
  - Engage user community for requirements
  - Define components and interface
  - Engage library developers

- Develop offgas subsystem component
  - Unit ops modeling
  - Separations and Waste Form Campaign off-gas "Sigma" team

Middle Tier

Bottom-up



- Ligand design
  - Incorporate QM energy scoring
  - Separations and Waster Form Campaign minor actinide "Sigma" team